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NEWS 9 Jul 12 BEILSTEIN enhanced with new display and select options, resulting in a closer connection to BABS  
NEWS 10 Jul 30 BEILSTEIN on STN workshop to be held August 24 in conjunction with the 228th ACS National Meeting  
NEWS 11 AUG 02 IFIPAT/IFIUDB/IFICDB reloaded with new search and display fields  
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NEWS 13 AUG 02 STN User Update to be held August 22 in conjunction with the 228th ACS National Meeting  
NEWS 14 AUG 02 The Analysis Edition of STN Express with Discover! (Version 7.01 for Windows) now available  
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NEWS 16 AUG 27 BIOCOMMERCE: Changes and enhancements to content coverage  
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NEWS 20 SEP 01 New display format, HITSTR, available in WPIDS/WPINDEX/WPIX  
  
NEWS EXPRESS JULY 30 CURRENT WINDOWS VERSION IS V7.01, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004  
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NEWS LOGIN Welcome Banner and News Items  
NEWS PHONE Direct Dial and Telecommunication Network Access to STN  
NEWS WWW CAS World Wide Web Site (general information)

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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 16:22:28 ON 08 SEP 2004

=> file hcaplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'HCAPLUS' ENTERED AT 16:22:35 ON 08 SEP 2004  
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FILE COVERS 1907 - 8 Sep 2004 VOL 141 ISS 11  
 FILE LAST UPDATED: 7 Sep 2004 (20040907/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

```
=> s iron {} overload {} disease?
      894883 IRON
      11168 IRONS
      895660 IRON
          (IRON OR IRONS)
      9126 OVERLOAD
      584 OVERLOADS
      9474 OVERLOAD
          (OVERLOAD OR OVERLOADS)
      801762 DISEASE?
L1      75 IRON (W) OVERLOAD (W) DISEASE?
```

```
=> s l1s l1 and chelator?
MISSING OPERATOR L1S L1
The search profile that was entered contains terms or
nested terms that are not separated by a logical operator.
```

```
=> s l1 and chelator?
      13655 CHELATOR?
L2      21 L1 AND CHELATOR?
```

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=> s l2 and review/dt
      1755763 REVIEW/DT
L3      6 L2 AND REVIEW/DT
```

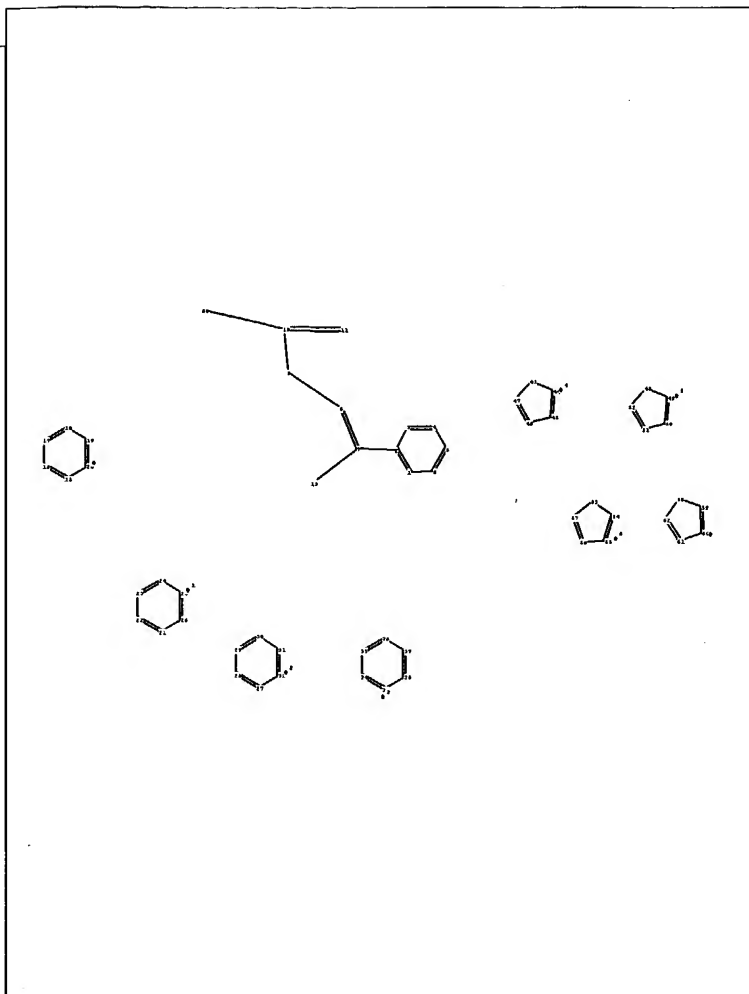
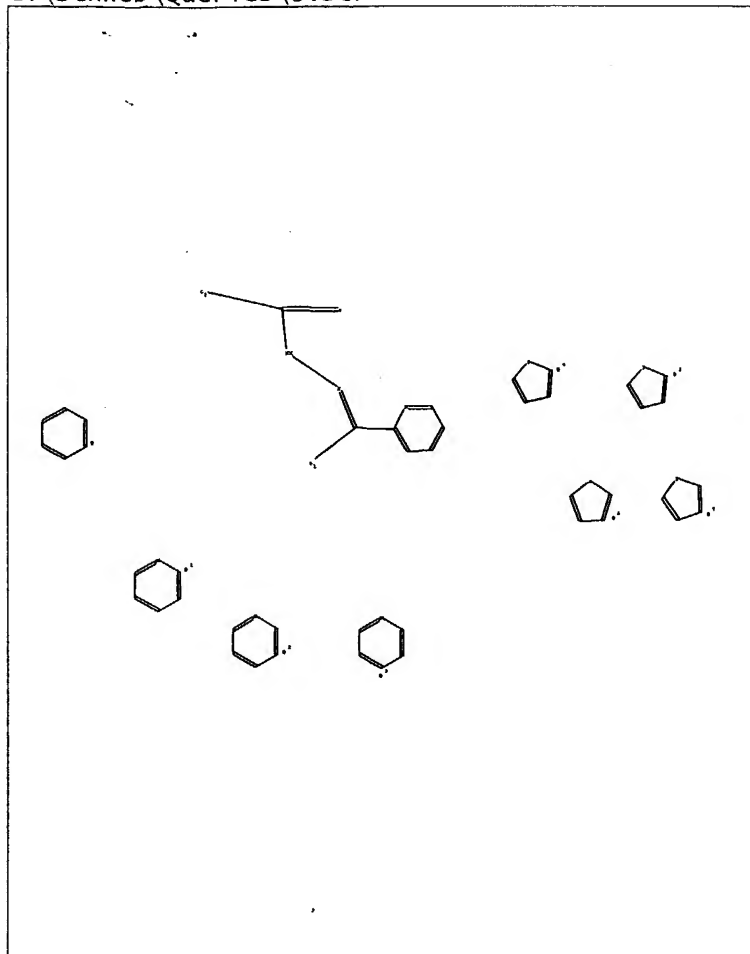
```
=> d l3, ibib abs, 1-6
```

L3 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Links
References	

ACCESSION NUMBER:	2004:136051 HCAPLUS
DOCUMENT NUMBER:	140:280599
TITLE:	Iron(III) <b>chelators</b> and thalassemia
AUTHOR(S):	Kumar, Praveen
CORPORATE SOURCE:	Department of Chemistry, Narain (P.G.) College, Shikohabad, 205 135, India

C:\stnweb\Queries\3.str



chain nodes :

7 8 9 10 11 13 68

ring nodes :

1 2 3 4 5 6 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32  
33 34 35 36 37 38 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58  
59 60 61 62

chain bonds :

2-7 7-8 7-13 8-9 9-10 10-11 10-68

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 15-16 15-20 16-17 17-18 18-19 19-20 21-22 21-26  
22-23 23-24 24-25 25-26 27-28 27-32 28-29 29-30 30-31 31-32 33-34 33-38 34-35  
35-36 36-37 37-38 43-44 43-47 44-45 45-46 46-47 48-49 48-52 49-50 50-51 51-52  
53-54 53-57 54-55 55-56 56-57 58-59 58-62 59-60 60-61 61-62

exact/norm bonds :

7-8 7-13 8-9 9-10 10-11 10-68 43-44 43-47 44-45 45-46 46-47 48-49 48-52  
49-50 50-51 51-52 53-54 53-57 54-55 55-56 56-57 58-59 58-62 59-60 60-61 61-62

exact bonds :

2-7

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 15-16 15-20 16-17 17-18 18-19 19-20 21-22 21-26  
22-23 23-24 24-25 25-26 27-28 27-32 28-29 29-30 30-31 31-32 33-34 33-38 34-35  
35-36 36-37 37-38

isolated ring systems :

containing 1 : 15 : 21 : 33 :

G1:H,OH

G2:[\*1],[\*2],[\*3],[\*4],[\*5],[\*6],[\*7]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS  
11:CLASS 13:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom  
22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom  
32:Atom

	33:Atom	34:Atom	35:Atom	36:Atom	37:Atom	38:Atom	43:Atom	44:Atom	45:Atom
46:Atom	47:Atom	48:Atom	49:Atom	50:Atom	51:Atom	52:Atom	53:Atom	54:Atom	55:Atom
56:Atom	57:Atom	58:Atom	59:Atom	60:Atom	61:Atom	62:Atom	68:CLASS		

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=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

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0.21

FILE 'REGISTRY' ENTERED AT 18:13:41 ON 08 SEP 2004  
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STRUCTURE FILE UPDATES: 7 SEP 2004 HIGHEST RN 741217-26-5  
 DICTIONARY FILE UPDATES: 7 SEP 2004 HIGHEST RN 741217-26-5

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when  
 conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more  
 information enter HELP PROP at an arrow prompt in the file or refer  
 to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR

=> s l1

SAMPLE SEARCH INITIATED 18:18:33 FILE 'REGISTRY'  
 SAMPLE SCREEN SEARCH COMPLETED - 16 TO ITERATE

100.0% PROCESSED 16 ITERATIONS 2 ANSWERS  
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 80 TO 560  
 PROJECTED ANSWERS: 2 TO 124

L2 2 SEA SSS SAM L1

=> s l1 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS  
 DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y  
 FULL SEARCH INITIATED 18:18:37 FILE 'REGISTRY'  
 FULL SCREEN SEARCH COMPLETED - 420 TO ITERATE

100.0% PROCESSED 420 ITERATIONS 18 ANSWERS  
 SEARCH TIME: 00.00.01

L3 18 SEA SSS FUL L1

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	158.36	158.57

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FILE COVERS 1907 - 8 Sep 2004 VOL 141 ISS 11  
 FILE LAST UPDATED: 7 Sep 2004 (20040907/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13

L4 6 L3

=> s 14 and richardson, d?/au

1214 RICHARDSON, D?/AU

L5 0 L4 AND RICHARDSON, D?/AU

=> s 14 and bernhardt, p?/au

253 BERNHARDT, P?/AU

L6 0 L4 AND BERNHARDT, P?/AU

=> s 14 and becker, e?/au

1294 BECKER, E?/AU

L7 0 L4 AND BECKER, E?/AU

=> d 14, ibib abs fhitstr, 1--6

L4 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text    **Listing**  
 References

ACCESSION NUMBER: 2003:610433 HCAPLUS  
 DOCUMENT NUMBER: 139:164699  
 TITLE: Preparation of 2-furancarboxylic acid hydrazides as glucagon antagonists  
 INVENTOR(S): Fujii, Akihito; Negoro, Toshiyuki; Migihashi, Chiaki; Murata, Makoto; Nakamura, Keiji; Nukuda, Takashi; Matsumoto, Takafumi; Konno, Kiyomi  
 PATENT ASSIGNEE(S): Dainippon Pharmaceutical Co., Ltd., Japan  
 SOURCE: PCT Int. Appl., 149 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2003064404	A1	20030807	WO 2003-JP871	20030130
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.:

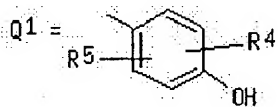
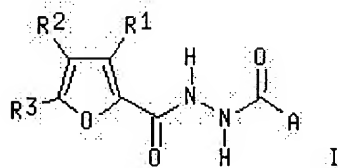
JP 2002-26012

A 20020201

OTHER SOURCE(S):

MARPAT 139:164699

GI



AB The title compds. I [A is Q1, etc.; one of R4 and R5 is cyano, nitro, etc., and the other is hydrogen, etc.; one of R1 and R2 is aryl, etc., and the other is hydrogen, aryl, etc.; R3 is hydrogen, etc.] are prepd. I exhibit potent glucagon receptor antagonism and are useful as preventive and/or therapeutic drugs for symptoms and diseases in which glucagon participates. In an in vitro test for glucagon receptor antagonism using a rat liver prepn., compds. of this invention showed IC50 values of 1.5 nM to 380 nM.

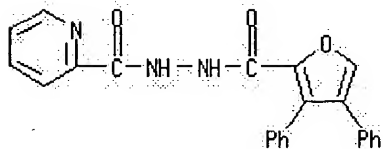
IT 576168-33-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of 2-furancarboxylic acid hydrazides as glucagon antagonists)

RN 576168-33-7 HCAPLUS

CN 2-Pyridinecarboxylic acid, 2-[(3,4-diphenyl-2-furanyl)carbonyl]hydrazide (9CI) (CA INDEX NAME)



REFERENCE COUNT:

1

THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text  
Citing References

ACCESSION NUMBER:

1980:550093 HCAPLUS

DOCUMENT NUMBER:

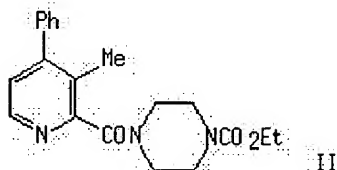
93:150093

TITLE:

Transformations in the pyridine series. A simple preparation of 3-methyl-4-phenylpyridine and corresponding 2-carboxamides



AUTHOR(S): Harrison, Ernest A., Jr.; Rice, Kenner C.; Rogers, Michael E.  
 CORPORATE SOURCE: Natl. Inst. Arthritis Metab. Dig. Dis., NIH, Bethesda, MD, 20205, USA  
 SOURCE: Heterocycles (1980), 14(6), 813-16  
 CODEN: HTCYAM; ISSN: 0385-5414  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



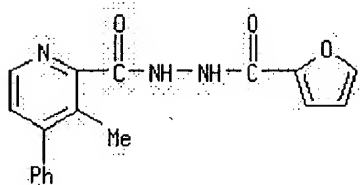
AB 3-Methyl-4-phenylpyridine (I) was prepd. in 96% yield by Huang-Minlon redn. of 4-phenyl-3-pyridinecarboxaldehyde. I was carboxylated followed by amidation to give its 1-pyridinecarboxamides, e.g. II. At 30 mg/kg II reduced edema in the rat adjuvant arthritis test by 17%.

IT 74834-52-9P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)

RN 74834-52-9 HCAPLUS

CN 2-Pyridinecarboxylic acid, 3-methyl-4-phenyl-, 2-(2-furanylcarbonyl)hydrazide, monohydrobromide (9CI) (CA INDEX NAME)



# HBr

L4 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Reference

ACCESSION NUMBER: 1974:551869 HCAPLUS

DOCUMENT NUMBER: 81:151869

TITLE: Heterocyclic compounds. XXII. Synthesis of 3,4-dihydroxy-2,5-dicarbomethoxyfuran derivatives. 2

AUTHOR(S): Yoshina, Shigetaka; Yamamoto, Katsumi

CORPORATE SOURCE: Fac. Pharm., Meijo Univ., Nagoya, Japan

SOURCE: Yakugaku Zasshi (1974), 94(9), 1139-48

CODEN: YKKZAJ; ISSN: 0031-6903

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

AB 3,4-Diaroyloxy-2,5-furancarboxylic acid hydrazides were prepd. by reaction of di-Me 3,4-diaroyloxy-2,5-furandicarboxylate derivs. with N<sub>2</sub>H<sub>4</sub>. 3,4-dimethoxy-2,5 furancarboxamide was similarly obtained. The hydrazides were treated with aldehydes to form hydrazones (28 compds.). Mass spectra were measured for the di-Me 3,4-diaroyloxy-2,5-furandicarboxylate derivs. and the hydrazides, and their fission pattern was examd. Uv absorption

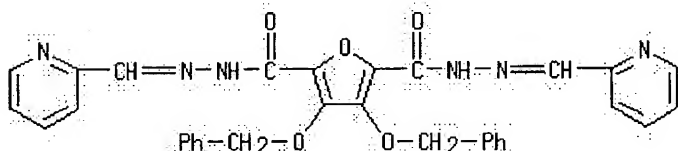
spectra of di-Me 3,4-diaroyloxy-2,5-furandicarboxylates and di-Me 3,4-dihydroxy-2,5-furandicarboxylate were also examd.

IT **53996-26-2P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN **53996-26-2** HCAPLUS

CN 2,5-Furandicarboxylic acid, 3,4-bis(phenylmethoxy)-, bis[(2-pyridinylmethylene)hydrazide] (9CI) (CA INDEX NAME)



L4 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text References

ACCESSION NUMBER: 1970:100448 HCAPLUS

DOCUMENT NUMBER: 72:100448

TITLE: Furan derivatives. XXXVIII. Hydrazidohydrazones of the pyridine and furan series

AUTHOR(S): Mndzhoyan, A. L.; Afrikyan, V. G.; Oganessian, R. S.; Adzhibekyan, A. S.; Karagezyan, S. G.; Sarafyan, V. G.

CORPORATE SOURCE: Inst. Tonkoi Org. Khim., Erevan, USSR

SOURCE: Armyanskii Khimicheskii Zhurnal (1969), 22(10), 922-32  
CODEN: AYKZAN; ISSN: 0515-9628

DOCUMENT TYPE: Journal

LANGUAGE: Russian

GI For diagram(s), see printed CA Issue.

AB A new series of title compds. was prepd. as potential chemotherapeutic agents for tuberculosis. To increase water soly. of the formerly prepd. analogs (CA 70: 1153 u; 67: 53943z), a new series (I) contg. morpholinomethyl (Q), piperidinomethyl (T), and pyrrolidinomethyl (Y) groups was obtained. R, R1, pyridyl ring, substitution position, % yield, and m.p. for I were as follows: Q, H, 2, 73, 150-1°; Q, H, 3, 70, 142-4°; Q, H, 4, 75.4, 157-8°; T, H, 2, 70, 146-8°; T, H, 3, 93, 161-2°; T, H, 4, 93, 168-9°; Y, H, 2, 92.7, 141-2°; Y, H, 3, 96, 109-10°; Y, H, 4, 92, 135-6°; 3,4-(MeO)2C6H3CH2 (Z), H, 2, 89.7, 140-1°; Z, H, 3, 88, 153-4°; Z, H, 4, 84.6, 226-7°; Me, Q, 2, 90, 112-13°; Me, Q, 3, 92, 109-10°; Me, Q, 4, 91, 125-6°; Me, T, 2, 89, 106-7°; Me, T, 3, 92, 127-8°; Me, T, 4, 92.2, 117-18°; Me, Y, 2, 92, 114-15°; Me, Y, B, 93, 111-12°; and Me, Y, 4, 91.7, 100-1°. II were also prepd. (same data given): Z, H, 2, 81.6, 187-8°; Z, H, 3, 87.5, 181-2°; Z, H, 4, 82, 158-9°; Z, Me, 2, 87.6, 148-50°; Z, Me, 3, 81, 145-6°; and Z, Me, 4, 89, 151-2°. In III, the substitution position of the pyridyl rings, % yield, and m.p. were: 2, 92.3, 248-9°; 3, 91, 300-1°; and 4, 93.8, 305-6°. Bactericidal potencies of the compds. against 8 tuberculosis lab. strains, in vitro, were low, except for 4 more active II with 2 and 4-pyridine orientation. Data on potencies and LD (for mice) of I, II, and III are given. I were 5-10 times more potent against a resistant strain, freshly obtained from patients, than against lab. strain. Phys. consts. of the intermediate furans were given. Prepns. were by conventional methods.

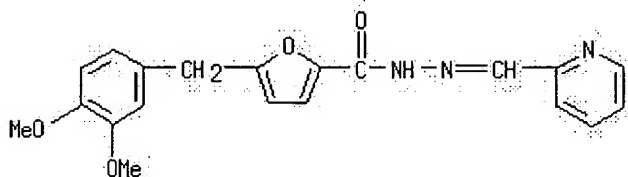
IT **26095-25-0P**

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

RN 26095-25-0 HCAPLUS

CN 2-Furoic acid, 5-veratryl-, (2-pyridylmethylene)hydrazide (8CI) (CA INDEX NAME)



L4 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Chemical Abstracts
-----------	--------------------

ACCESSION NUMBER: 1969:11530 HCAPLUS

DOCUMENT NUMBER: 70:11530

TITLE: Furan derivatives. XXXIII.  $\alpha$ -,  $\beta$ -, and  $\gamma$ -Pyridinecarboxaldehyde 5-and 4,5-substituted furoylhydrazones

AUTHOR(S): Mndzhoyan, A. L.; Afrikyan, V. G.; Oganessian, R. S.; Shakhmuradova, A. O.; Zhuruli, L. D.; Karagezyan, S. G.; Sarafyan, V. G.

CORPORATE SOURCE: Inst. Tonkoi Org. Khim., Erevan, USSR

SOURCE: Armyanskii Khimicheskii Zhurnal (1968), 21(4), 340-7  
CODEN: AYKZAN; ISSN: 0515-9628

DOCUMENT TYPE: Journal

LANGUAGE: Russian

GI For diagram(s), see printed CA Issue.

AB The following hydrazides (I) of 5- and 4,5-substituted furan-2-carboxylic acids were prepd. by boiling 0.1 mole of an alkyl ester of the acid with 0.12 mole  $N_2H_4 \cdot H_2O$  in abs. EtOH for 10 hrs. (R, R', % yield, and m.p. given): Me, H, 96.1, 59-60°; Et, H, 78.0, 68-70°; PhCH<sub>2</sub>, H, 91.1, 98-9°; MeC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>, H, 94, 104-5°; MeOC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>, H, 88.1, 80-2°; Me, Me, 80.0, 95-6°; Me, PhCH<sub>2</sub>, 79.5, 109-10°.

Treatment of 0.1 mole I with 0.11 mole  $\alpha$ -,  $\beta$ - and  $\gamma$ -pyridine-carboxaldehyde, resp., in abs. EtOH yielded the following II R, R', orientation of pyridine ring, % yield, and m.p. given): Me, H,  $\alpha$ , 78.8, 178-9°; Me, H,  $\beta$ , 91.3, 129-30°; Me, H,  $\gamma$ , 89.9, 150-1°; Et, H,  $\alpha$ , 75.8, 138-9°; Et, H,  $\beta$ , 90.9, 163-4°; Et, H,  $\gamma$ , 89.8, 115-16°; PhCH<sub>2</sub>, H,  $\alpha$ , 89.3, 164-5°; PhCH<sub>2</sub>, H,  $\beta$ , 95.5, 195-6°; PhCH<sub>2</sub>, H,  $\gamma$ , 95.3, 175-6°; MeC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>, H,  $\alpha$ , 68.4, 135-7°; MeC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>, H,  $\beta$ , 80.0, 155-6°; MeC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>, H,  $\gamma$ , 78.0, 176-8°; MeOC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>, H,  $\alpha$ , 70.0, 164-5°; MeOC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>, H,  $\beta$ , 60.4, 185-6°; MeOC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>, H,  $\gamma$ , 75.5, 170-1°; Me, Me,  $\alpha$ , 72.5, 189-90°; Me, Me,  $\beta$ , 94.0, 180-2°; Me, Me,  $\gamma$ , 83.0, 175-6°; Me, PhCH<sub>2</sub>,  $\alpha$ , 75.6, 184-5°; Me, PhCH<sub>2</sub>,  $\beta$ , 94.6, 162-3°; Me, PhCH<sub>2</sub>,  $\gamma$ , 81.8, 180-1°. Reaction of pyridinecarboxaldehydes with the hydrazides of pyridinecarboxylic acids generated the following III (orientation of acid, orientation of aldehyde, % yield, and m.p. given):  $\alpha$ ,  $\alpha$ , 91.6, 158-9°;  $\alpha$ ,  $\beta$ , 90.6, 168-9°;  $\alpha$ ,  $\gamma$ , 74.8, 194-5°;  $\beta$ ,  $\alpha$ , 71.2, 158-9°;  $\beta$ ,  $\beta$ , 80.0, 206-7°;  $\beta$ ,  $\gamma$ , 68.6, 197-8°;  $\gamma$ ,  $\alpha$ , 70.1, 163-4°;  $\gamma$ ,

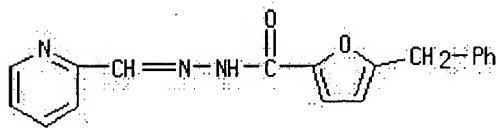
$\beta$ , 72.2, 233-4°;  $\gamma$ ,  $\gamma$ , 83.1, 227-9°. IV were also prepd. (no chem. details given). All compds. were tested for tuberculostatic activity against several strains of organisms. Of all compds., those most generally effective were those members of groups III and IV which were derived from pyridine-2- and pyridine-4-carboxylic acid.

IT 20842-30-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 20842-30-2 HCAPLUS

CN 2-Furoic acid, 5-benzyl-, (2-pyridylmethylene)hydrazide (8CI) (CA INDEX NAME)



L4 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text References

ACCESSION NUMBER: 1967:453943 HCAPLUS

DOCUMENT NUMBER: 67:53943

TITLE: Furan derivatives. XXXI. Some acid 2-alkylidene hydrazides and N,N'-diacylhydrazines as potential antitubercular agents

AUTHOR(S): Mndzhoyan, A. L.; et al.

SOURCE: Armyanskii Khimicheskii Zhurnal (1966), 19(10), 793-805

CODEN: AYKZAN; ISSN: 0515-9628

DOCUMENT TYPE: Journal

LANGUAGE: Russian

GI For diagram(s), see printed CA Issue.

AB cf. CA 63: 18004h. The title compds. were synthesized to find active antitubercular agents. 4-Ethoxybenzyl chloride (I), b1 105°, was prepd. in 67.7% yield by chloromethylation of phenetole. To 40 g. Me furan-2-carboxylate in 50 ml. CS<sub>2</sub> in the presence of 0.025 mole ZnCl<sub>2</sub>, 10 ml. I in 50 ml. CS<sub>2</sub> was added dropwise with stirring at 0° and the mixt. kept 30 min. at 0° and 30 min. at room temp. to give Me 5-(p-ethoxybenzyl)furan-2-carboxylate. Similarly prepd. were the following II, (R1 = H, R2 = CO<sub>2</sub>Me) (R, % yield, b.p./mm., n<sub>20</sub>D, and d<sub>20</sub> given): p-ClC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>, 61.3, 178-9°/3 (m. 36-7°), -, -; p-MeOC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>, 50.5, 176-8°/3, 1.1704, 1.5588; p-EtOC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>, 46.8, 183-5°/3, 1.1475, 1.5475; p-PrOC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>, 50.2, 189-90°/3, 1.1232, 1.5435; p-BuOC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>, 51.5, 196-8°/3, 1.1184, 1.5420; p-AmOC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>, 49.2, 210-11°/3, 1.0992, 1.5368. Similarly prepd. was 85.2% II (R = Me, R1 = PhCH<sub>2</sub>, R2 = CO<sub>2</sub>Me), b2 161-2°, n<sub>20</sub>D 1.4110, d<sub>20</sub> 1.5542. Sapon. of II (R1 = H, R2 = CO<sub>2</sub>Me) with 10% KOH gave the following II (R1 = H, R2 = CO<sub>2</sub>H) (R, % yield, and m.p. given): p-ClC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>, 90.3, 98-9°; p-MeOC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>, 83.4, 124-5°; p-EtOC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>, 85.3, 148-9°; p-PrOC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>, 82.3, 111-12°; p-BuOC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>, 83.5, 125-6°; p-AmOC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>, 81.4, 117-18°. Similarly prepd. was 90.3% II (R = Me, R1 = PhCH<sub>2</sub>, R2 = CO<sub>2</sub>H), m. 134-5°. Decarboxylation of II (R2 = CO<sub>2</sub>H) carried out at 190-250° gave the following II (R2 = H) (R, R1, % yield, b.p./mm., n<sub>20</sub>D, and d<sub>20</sub> given): p-ClC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>, H, 93.9, 119-20°/3, 1.4482, 1.1189; p-MeOC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>, H, 81.5, 122-3°/2, 1.5484, 1.1065; p-EtOC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>, H, 90.4, 123-5°/2, 1.5400, 1.0683; p-PrOC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>, H, 92.8, 135-6°/2, 1.5330, 1.0519; p-BuOC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>, H, 94.5,

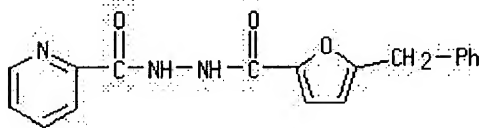
142-4°/2, 1.5278, 1.0355; p-AmOC6H4CH2, H, 90.5, 151-3/2, 1.5238, 1.0239; Me, PhCH2, 89.5, 122-4°/15, 1.5415, 0.9871. From disubstituted furan was obtained the 4-benzyl-5-methyl deriv. which also was decarboxylated. The 5- and 4,5-substituted furans were formylated and acetylated. Formylation was accomplished by methods previously described (CA 59: 2763g). To 0.15 mole Me2NCHO at 0°, 0.15 mole POCl3 was added slowly with stirring. The mixt. was stirred 30 min. at 0°, 0.1 mole freshly distd. 2-ethoxybenzylfuran was added at 10° during 0.5 hr., and the mixt. kept in an ice bath 30 min., poured into 200 ml. ice water at room temp., neutralized with Na2CO3, and kept overnight to give the following II (R2 = CHO) (R, R1, % yield, b.p./mm., m.p., n20D, and d20 given): p-ClC6H4CH2, H, 73.4, 176-8°/3, 39-40, -, -; p-MeOC6H4CH2, H, 72.5, 190-2°/3, -, 1.5904, 1.1767; p-EtOC6H4CH2, H, 81.5, 186-8°/3, -, 1.5768, 1.1930; p-PrOC6H4CH2, H, 79.7, 208-10°/3, 37-8°, -, -; p-BuOC6H4CH2, H, 81.2, 190-2°/3, 42-3°, -, -; p-AmOC6H4CH2, H, 80.7, 198-9°/3, 44-6°, -, -; Me, PhCH2, 87.5, 171-2°/5, -, 1.5869, 1.1182. To 0.1 mole freshly distd. 5-(p-ethoxybenzyl)furan and 0.2 mole Ac2O at 0°, H3PO4 was added with stirring and the mixt. stirred 30 min. and heated on a boiling water bath 3 hrs. to give the following II (R2 = Ac) (R, R1, % yield, b.p./mm., m.p., n20D, and d20 given): p-ClC6H4CH2, H, 70.3, 171-2°/2, 34-5°, -, -; p-MeOC6H4CH2, H, 50.3, 191-2°/2, -, 1.5750, 1.1405; p-EtOC6H4CH2, H, 51.8, 175-8°/2, -, 1.6502, 1.1283; p-PrOC6H4CH2, H, 63.2, 185-7°/2, -, 1.5558, 1.1177; p-BuOC6H4CH2, H, 65.5, 189-90°/2, -, 1.5598, 1.0909; p-AmOC6H4CH2, H, 67.1, 193-5°/2, 48-50°, -, -; Me, PhCH2, 40.7, 163-5°/2, -, 1.5720, 1.1011. The III listed in the first table were obtained by action of the appropriate pyridinecarboxylic acid hydrazide on the substituted furfural or substituted 2-acetylfuran in an alc. medium. From equimol. amts. of 5-methyl-4-benzylfuran-2-carbonyl chloride and picolinic acid hydrazide in 60 ml. dry pyridine heated at 120° for 10 hrs. were obtained the IV listed in the second table. [TABLE OMITTED] To equimol. amts. of the HCl salt, the chloride, and the hydrazide of picolinic acid, 7-g. KOH in 200 ml. EtOH was added with stirring and the mixt. heated 10 hrs. to give the following RCONHNHCOR1 (R, R1, % yield, and m.p. given): α-C5H4N, α-C5H4N, 37.1, 127-9°; α-C5H4N, β-C5H4N, 35.2, 215-16°; α-C5H4N, γ-C5H4N, 16.9, 208-9°; β-C5H4N, β-C5H4N, 25.6, 208-10°; β-C5H4N, γ-C5H4N, 20.2, 185-7°; γ-C5H4N, γ-C5H4N, 17.5, 196-8°. [TABLE OMITTED] Tubercular activity was tested in vitro. The most active compds. were derivs. of isonicotinic acid pyridinecarboxylic acids.

IT **15033-03-1P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN **15033-03-1** HCAPLUS

CN Hydrazine, 1-(5-benzyl-2-furoyl)-2-picolinoyl- (8CI) (CA INDEX NAME)



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